Freezing transition in a direction-free kinetically constrained model on a finite dimensional lattice

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Abstract. - We propose a direction-free kinetically constrained model on the square lattice and show that this model exhibits a freezing transition at a non-trivial density. By numerical experiments, we also conjecture that critical exponents characterizing the singular behaviour near the transition point are different from those of previously known freezing transitions in finite dimensions.

Introduction. – Athermal particles with repulsive interactions exhibit rigidity with an amorphous structure when the density of the particles is higher than a critical value. Such a phenomenon is referred to as a *jamming transition*, and elucidation of the nature of jamming transitions is a challenging problem in statistical physics [1–8]. Thus far, the replica theory in equilibrium statistical mechanics has provided an insight into jamming transitions as well as glass transitions [9, 10]. As a different approach, kinetically constrained models (KCMs), which were investigated with a physical picture that glassy dynamics is purely kinematic [11], have been considered for understanding jamming transitions [12]. A notable property of KCMs is the absence of singularities in the equilibrium properties. Although KCMs are simple mathematical models that lack several properties of realistic materials, recent experimental studies have attempted to reveal the relationship between KCMs and glass-forming materials [13, 14].

Let us review theoretical studies on KCMs in brief. The first rigorous proof for the existence of a freezing transition was presented for the Fredrickson-Andersen model and the Kob-Andersen model on a Bethe lattice [15]. In this case, a freezing transition means a transition to a freezing phase where an infinite number of particles are at rest as a result of blocking by other particles. However, for these models in finite dimensions, it has been shown that there are no true phase transitions [16, 17], even though the results of numerical simulations suggested the existence of transition. Then, a remarkable discovery was made that certain KCMs exhibit a freezing transition in two dimensions [12, 18–20]. Here, it should be noted that the constraint conditions of these models depend on directions. This characteristic property of KCMs distinguishes them from the more familiar *direction-free* models such as the Ising models.

The basic motivation in the present study is to establish the idea of universality classes for freezing transitions observed in finite-dimensional KCMs. However, this problem cannot be considered directly, because such KCMs are scarcely found. Hence, we first need to collect examples of KCMs that exhibit a freezing transition in finite dimensions. In particular, because all the examples known thus far belong to the same universality class, which we refer to as *the Toninelli-Biroli-Fisher (TBF) class*, it is a significant challenge to present a KCM that does not belong to the TBF class, and exhibits a freezing transition despite this. We attempt to solve this problem.

In particular, we focus on direction-free KCMs, which may be conjectured as qualitatively different from KCMs in the TBF class because of the symmetry property related to directions. Direction-free models also present an advantage in that their mean-field analysis may be easier. Mean-field analysis acts as a starting point for a theory on determining the universality, as we have learned from the renormalization group analysis for equilibrium critical phenomena. Therefore, the discovery of a direction-free KCM that exhibits a freezing transition might be

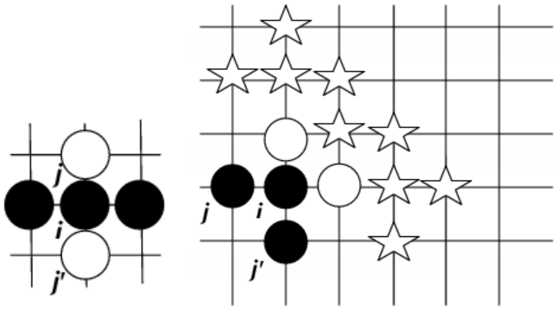

Fig. 1: Two configurations satisfying $\sum_{j\in \mathrm{B}_i}\sigma_j = 2$. In the configuration to the left, the particle at site i is constrained, because f_j and $f_{j'}$ are at most 1. In the configuration to the right, the particle at site i is not constrained when there are no particles at the sites marked with the star symbol. The particle at site i becomes constrained when a particle is placed at the sites marked with the star symbol.

useful for further studies on the universality. With this background, we propose a direction-free two-dimensional KCM for which the existence of a freezing transition can be proved rigorously. We also conjecture by numerical experiments that the proposed model does not belong to the TBF class.

Model. – Let Λ be a square lattice consisting of sites $i \equiv (i_x, i_y)$, where i_x and i_y are integers satisfying $1 \le i_x \le L$ and $1 \le i_y \le M$. We assume $M \le L$ without loss of generality. We define the occupation variable $\sigma_i \in \{0,1\}$ at each site $i \in \Lambda$, and we assume a simple Hamiltonian

$$H(\boldsymbol{\sigma}) = \sum_{i\in\Lambda}\sigma_i, \tag{1}$$

where we express $\boldsymbol{\sigma} \equiv (\sigma_i)_{i\in\Lambda}$ collectively. Concretely, $\sigma_i = 1$ represents a state that a particle occupies site i, while there is no particle at site i when $\sigma_i = 0$. In the argument below, we assume that particles are filled outside the system unless otherwise mentioned explicitly.

We consider a Markov stochastic process with a transition ratio $R(\boldsymbol{\sigma} \to \boldsymbol{\sigma}')$ for $\boldsymbol{\sigma} \ne \boldsymbol{\sigma}'$. Let $P(\boldsymbol{\sigma}, t)$ be the probability distribution of a particle configuration $\boldsymbol{\sigma}$ at time t. The time evolution of $P(\boldsymbol{\sigma}, t)$ obeys

$$\partial_t P(\boldsymbol{\sigma}, t) = \sum_{\boldsymbol{\sigma}'\ne\boldsymbol{\sigma}}[R(\boldsymbol{\sigma}' \to \boldsymbol{\sigma})P(\boldsymbol{\sigma}', t) - R(\boldsymbol{\sigma} \to \boldsymbol{\sigma}')P(\boldsymbol{\sigma}, t)]. \tag{2}$$

In this work, we study a constrained Glauber dynamics, where the transition ratio $R(\boldsymbol{\sigma} \to \boldsymbol{\sigma}')$ is written as

$$R(\boldsymbol{\sigma} \to \boldsymbol{\sigma}') = \sum_i \delta(\boldsymbol{\sigma}', F_i\boldsymbol{\sigma}) r(\boldsymbol{\sigma} \to \boldsymbol{\sigma}')\mathcal{C}_i(\boldsymbol{\sigma}). \tag{3}$$

We explain the right-hand side of the equation in order. First, F_i is the creation and annihilation operator described by

$$(F_i\boldsymbol{\sigma})_j = (1-\sigma_i)\delta_{ij} + \sigma_j(1-\delta_{ij}). \tag{4}$$

The term $\delta(\boldsymbol{\sigma}', F_i\boldsymbol{\sigma})$ represents a rule that the transition is caused by a particle creation or annihilation at each site. The term $r(\boldsymbol{\sigma} \to \boldsymbol{\sigma}')$ is given as

$$r(\boldsymbol{\sigma} \to \boldsymbol{\sigma}') = \min\left[1, \exp\left(\frac{H(\boldsymbol{\sigma}) - H(\boldsymbol{\sigma}')}{T}\right)\right], \tag{5}$$

where it satisfies

$$\frac{r(\boldsymbol{\sigma} \to \boldsymbol{\sigma}')}{r(\boldsymbol{\sigma}' \to \boldsymbol{\sigma})} = \exp\left(-\frac{H(\boldsymbol{\sigma}') - H(\boldsymbol{\sigma})}{T}\right). \tag{6}$$

Finally, with regard to the function $\mathcal{C}_i(\boldsymbol{\sigma})$, $\mathcal{C}_i(\boldsymbol{\sigma}) = 0$ specifies a set of configurations for which particle creation and annihilation at site i is prohibited, and $\mathcal{C}_i(\boldsymbol{\sigma}) = 1$, for the other configurations. We also assume that $\mathcal{C}_i(\boldsymbol{\sigma})$ is independent of σ_i.

It should be noted that the canonical distribution with the Hamiltonian (1) is the stationary solution of (2) with (3) because the transition ratio (3) satisfies the detailed balance condition. Therefore, there are no equilibrium phase transitions in the system. Nevertheless, it has been shown that there is another steady state (a freezing state) for an appropriately selected $\mathcal{C}_i(\boldsymbol{\sigma})$, which is different from the equilibrium steady state. All examples of such $\mathcal{C}_i(\boldsymbol{\sigma})$ known thus far depend on directions [16, 18, 20]. In contrast to those in the previous cases, we propose a direction-free function $\mathcal{C}_i(\boldsymbol{\sigma})$ that leads to a freezing state, where, in precise terms, a direction-free $\mathcal{C}_i(\boldsymbol{\sigma})$ should be expressed only in terms of B_j, which indicates the set of sites connected to site j in the lattice Λ.

Now, we explain our selection of $\mathcal{C}_i(\boldsymbol{\sigma})$. We first define

$$f_i \equiv \sum_{j\in \mathrm{B}_i}\delta(\sigma_j, 0)\left[\prod_{\ell\in \mathrm{B}_j}\delta(\sigma_\ell, 0)\right], \tag{7}$$

where $\delta(m, n)$ represents Kronecker's delta function. For site i, f_i represents the number of empty sites j in B_i such that there are no particles next to any site j. From this definition, we find $f_i = 0$ for site i with a particle. Then, we set $\mathcal{C}_i(\boldsymbol{\sigma}) = 0$, only when (i) $\sum_{j\in \mathrm{B}_i}\sigma_j \ge 3$ or (ii) $\sum_{j\in \mathrm{B}_i}\sigma_j = 2$ and

$$\sum_{j\in \mathrm{B}_i}\delta(f_j, 2) \le 1. \tag{8}$$

Condition (i) is a standard constraint for KCMs, while the additional rule (8) in condition (ii) may appear unfamiliar. We explain rule (ii) through the following examples.

In figure 1, for the particle at site i, there are two cases satisfying the condition $\sum_{j\in \mathrm{B}_i}\sigma_j = 2$. In the configuration to left of the figure, f_j and $f_{j'}$, for the empty sites j and j', are at most 1. As $\sum_{j\in \mathrm{B}_i}\delta(f_j, 2) = 0$ in this case, $\mathcal{C}_i(\boldsymbol{\sigma}) = 0$. Throughout this work, we say that *the particle at site i is constrained* when $\mathcal{C}_i(\boldsymbol{\sigma}) = 0$ and $\sigma_i = 1$. On the other hand, in the configuration to the right in figure 1, when there are no particles at the sites marked with the star symbol, f_j and $f_{j'}$ for the empty sites j and j'

are 2, and consequently, $\sum_{j\in \mathrm{B}_i}\delta(f_j,2)=2$. In this case, the particle at site i is not constrained. When at least one particle is placed at the sites marked with the star symbol, $\sum_{j\in \mathrm{B}_i}\delta(f_j,2)=1$ and the particle at site i is constrained as the result. Using similar considerations, we also find that the function $\mathcal{C}_i(\boldsymbol{\sigma})$ is independent of σ_i.

In this work, we focus on the relaxation behaviours of the system from an initial state, where sites are randomly occupied with a probability ρ. Moreover, as the simplest case, we consider the zero temperature limit $T\to 0$. The equilibrium state in this case involves no particles. Now, let us suppose that a particle configuration at $t=0$ contains a set of particles constrained by only constrained particles. Such particles are referred to as *frozen particles.* Then, frozen particles cannot annihilate, and thus they can never reach the equilibrium state. We refer to this phenomenon as *freezing.* On the other hand, when no frozen particles exist at $t=0$, all the particles annihilate, and hence, the final state becomes the equilibrium state. In this manner, whether a freezing transition occurs is determined by investigating the existence of frozen particles in initial configurations.

Existence of a freezing transition. – In this section, we prove that a freezing transition occurs at some value $0<\rho_{\mathrm{c}}<1$ in the proposed model. In concrete terms, we show that there is a density $\rho_{\mathrm{l}}>0$, below which the probability of finding frozen particles in initial configurations is zero in the thermodynamic limit, while there is a density $\rho_{\mathrm{u}}<1$, above which frozen particles can be found in initial configurations with probability one in the thermodynamic limit. By estimating ρ_{l} and ρ_{u}, we may conclude that $0<\rho_{\mathrm{l}}\le\rho_{\mathrm{c}}\le\rho_{\mathrm{u}}<1$, which means that ρ_{l} and ρ_{u} are a lower bound and an upper bound of the transition point, respectively.

No frozen particles for $\rho<\rho_{\mathrm{l}}$. Let $(i^{(k)})_{k=1}^{N}$ be a sequence of N-sites such that (i) $\sigma_{i^{(k)}}=1$, (ii) $|i^{(k)}-i^{(k+1)}|\le 3$, and (iii) $|i^{(k)}-i^{(k')}|>3$ for $k'\neq k\pm 1$, where $|i-j|\equiv|i_x-j_x|+|i_y-j_y|$. For a given configuration $\boldsymbol{\sigma}$, we define a set of all such sequences, which is denoted by $\mathcal{D}_N(\boldsymbol{\sigma})$. Here, if frozen particles are present in the initial configuration $\boldsymbol{\sigma}$, we can always find a sequence of sites in $\mathcal{D}_{M/3}(\boldsymbol{\sigma})$. (Recall that $M\le L$.) Thus, the probability Q of finding frozen particles in initial conditions is less than $\mathrm{Prob}(\mathcal{D}_{M/3}\neq\phi)$. Here, the latter probability is less than $(24\rho)^{\frac{M}{3}}$, where 24 is the number of sites whose distance from one site is at most three. These estimations give $Q<(24\rho)^{\frac{M}{3}}$. When ρ is less than $1/24$, $Q\to 0$ in the thermodynamic limit. We thus find a lower bound as $\rho_{\mathrm{l}}=1/24$.

Frozen particles for $\rho>\rho_{\mathrm{u}}$. Let $\mathcal{B}$ be a set of oriented bonds written as $\{(4k,2l)\to(4k+2,2l\pm 1)\}$ or $\{(4k-2,2l+1)\to(4k,2l+1\pm 1)\}$, where $k,l\in\mathbb{Z}$. We say that a bond $\{(n,m)\to(n+2,m\pm 1)\}\in\mathcal{B}$ is occupied when three sites (n,m), $(n+1,m)$, and $(n+1,m\pm 1)$ are all occupied. Now, if there exists an infinite connected cluster (in the sense of a directed percolation) of the occupied bonds in $\mathcal{B}$, we can find frozen particles in the thermodynamic limit. The problem is similar to the standard directed percolation. However, the occupation of bond $\{(4k,2l)\to(4k+2,2l+1)\}$ is not independent of the occupation of bond $\{(4k,2l)\to(4k+2,2l-1)\}$ because the occupation of the two sites, $(4k,2l)$ and $(4k+1,2l)$, influences the two bonds.

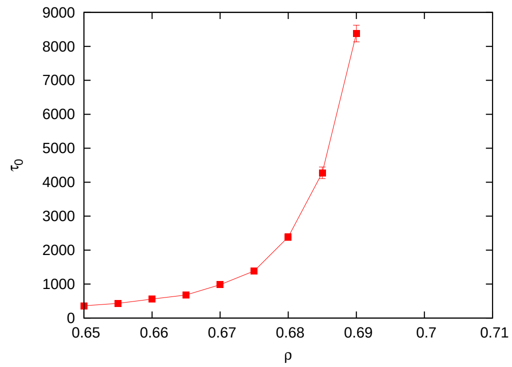

Fig. 2: Relaxation time τ_0 with $L=10000$.

In order to estimate the condition for the existence of an infinite connected cluster, we introduce two auxiliary variables, β_i^+ and β_i^-, which take the value 0 with probability $1-\tilde{\rho}$, and 1, with probability $\tilde{\rho}$. By using these variables, we may determine an initial configuration $\boldsymbol{\sigma}$ by using the relation $\sigma_i=\beta_i^++\beta_i^--\beta_i^+\beta_i^-$. The probability ρ is then related to $\tilde{\rho}$ as $\rho=1-(1-\tilde{\rho})^2$. Here, instead of the bond defined by the occupation variable σ_i, we consider the bond defined by the auxiliary variables $\beta_i^{\pm}$, as follows. We say that a bond $\{(n,m)\to(n+2,m+1)\}$ is β-occupied when $\beta_{n,m}^+=\beta_{n+1,m}^+=\beta_{n+1,m+1}^+=1$. Likewise, $\{(n,m)\to(n+2,m-1)\}$ is called β-occupied when $\beta_{n,m}^-=\beta_{n+1,m}^-=\beta_{n+1,m-1}^-=1$. As β-occupation for each bond independently occurs with the probability $p=\tilde{\rho}^3$, there is a critical value $p_{\mathrm{c}}=\tilde{\rho}_{\mathrm{c}}^3\simeq 0.644\cdots$, above which the directed bond percolation occurs [21]. If a bond is β-occupied, the bond is occupied. Thus, an infinite connected cluster of β-occupied bonds indicates an infinite connected cluster of bonds in the original problem. By setting $\rho_{\mathrm{u}}=1-(1-\tilde{\rho}_{\mathrm{c}})^2$, we find that there exists an infinite connected cluster (in the sense of a directed percolation) of occupied bonds in $\mathcal{B}$ for $\rho>\rho_{\mathrm{u}}$. This $\rho_{\mathrm{u}}\simeq 0.981\cdots$ is an upper bound of ρ_{c}.

Transition point and universality class. – In this section, with the aid of numerical experiments, we obtain greater lower bounds and smaller upper bounds of the transition point than the rigorous estimations given in the previous section. We also present evidence that the singular behaviour near the transition point is different from that for the TBF class.

Greater lower bounds. Lower bounds of the transition point are numerically obtained by checking whether initial

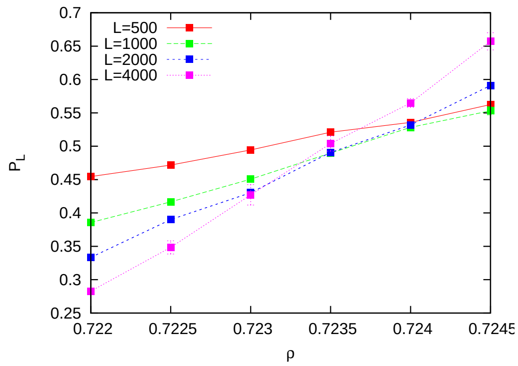

Fig. 3: $P_L(\rho)$ for $z^{-1} = 0.63$.

configurations with density ρ relax to the equilibrium configuration. To elaborate, we measure the relaxation time τ_0 when $H(\boldsymbol{\sigma})$ becomes 0 as a function of ρ. As shown in figure 2, τ_0 increases when ρ is increased. From the graph, we can claim that $\rho_c > 0.69$. Due to the rapid increase in τ_0 at high densities, a better numerical estimation of the lower bound becomes difficult.

Smaller upper bounds. The transition point is obtained from the thermodynamic limit of the probability of finding frozen particles in initial configurations. However, as discussed in the previous subsection, direct numerical estimation is practically impossible because the relaxation time becomes too long to distinguish between a slow relaxation process and a freezing state. Nevertheless, in order to know the upper bounds of the transition point, we simply require to observe a percolation of frozen particles in the direction from left to right under the boundary condition that particles are filled in the left- and right-side regions, while no particles exist in the top and bottom regions [22]. In fact, if such a directed percolation occurs in this modified system, frozen particles would be observed in the original system with the filled boundary conditions.

In order to detect a directed percolation, we numerically investigate the probability $P_L(\rho)$ of finding a frozen configuration in the modified system with $M = L^{1/z}$, where $0 < z^{-1} < 1$ because $M \leq L$. Then, for an assumed value of z, we determine whether a density $\rho_{\rm dp}$ exists such that $\lim_{L\to\infty} P_L(\rho) = \theta(\rho - \rho_{\rm dp})$, where $\theta(\ )$ is the Heaviside function. If such a density $\rho_{\rm dp}$ exists, it corresponds to a directed percolation point with the assumed value z. In this manner, we can determine a set of values $(\rho_{\rm dp}, z)$, and $\rho_{\rm dp}$ provides an upper bound of the transition point. Practically, in numerical experiments, for a given value of z, we consider a cross point of the two curves $P_{L/2}(\rho)$ and $P_L(\rho)$, which is denoted by $\rho_{\rm cr}^L(z^{-1})$. We then check whether or not $\rho_{\rm cr}^L(z^{-1}) \to \rho_{\rm dp}$ in the limit $L \to \infty$.

We first set $z^{-1} = 0.63$, which is the dynamical exponent of the standard directed percolation [21]. As shown in figure 3, the numerical data up to $L = 4000$ suggest that $\rho_{\rm cr}^L$ are too scattered to judge convergence to a special value where the density is changed by an increment of

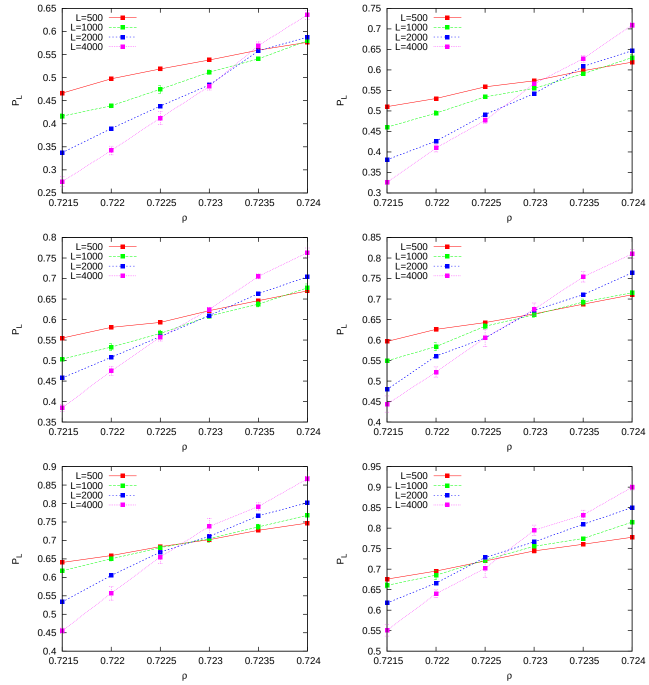

Fig. 4: $P_L(\rho)$ with $z^{-1} = 0.64$ and 0.65 (top), $z^{-1} = 0.66$ and 0.67 (middle), and $z^{-1} = 0.68$ and 0.69 (bottom).

0.0005. We thus seek the possibility of the convergence of $\rho_{\rm cr}^L$ for a different value of z^{-1}. Specifically, by changing z^{-1} with an increment of 0.01 from 0.63, we measured $P_L(\rho)$. The results for $0.64 \leq z^{-1} \leq 0.69$ are shown in figure 4. From the graphs, one may conjecture, for example, that a good convergence of $\rho_{\rm cr}^L$ is expected for $z^{-1} = 0.68$. We then quantitatively investigate the extent of the convergence by measuring the average value of the cross points $\bar{\rho}_{\rm cr} \equiv \sum_{i=1}^{3} \rho_{\rm cr}^{L_i}(z^{-1})/3$ with $L_i = 500 \times 2^i$ and the deviation $\Delta\rho_{\rm cr} \equiv \sqrt{\sum_{i=1}^{3}(\rho_{\rm cr}^{L_i} - \bar{\rho}_{\rm cr})^2/3}$ for each value of z^{-1}. Here, we estimated $\rho_{\rm cr}^{L_i}$ by approximating $P_L(\rho)$ as a piece-wise linear function. When $\Delta\rho_{\rm cr}$ is sufficiently small, we expect an obvious convergence of $\rho_{\rm cr}^L(z^{-1})$ in the limit $L \to \infty$.

Figure 5 presents the numerical results of $\Delta\rho_{\rm cr}$ for $0.63 \leq z^{-1} \leq 0.78$, where $\Delta\rho_{\rm cr}$ exhibits an oscillatory behaviour. Such a behaviour has never been reported. Here, we assume that the local minima in $\Delta\rho_{\rm cr}$ provide convergence points, by relying on the interpretation that the existence of such multi-convergence points implies the coexistence of different types of directed percolations with different exponents z at different densities $\rho_{\rm dp}$. This leads to the conclusion that the convergence points are $z^{-1} = 0.64, 0.68, 0.73$, and 0.75, within numerical accuracy. The corresponding values of $\rho_{\rm dp}$ are displayed in figure 6. We also conjecture that there are more convergence points at a larger value of z^{-1}, even though it is not easy to obtain them numerically due to the longer numerical simulations required. In principle, there exists a least upper bound $\rho_{{\rm dp}*}$, that can be obtained by this procedure,

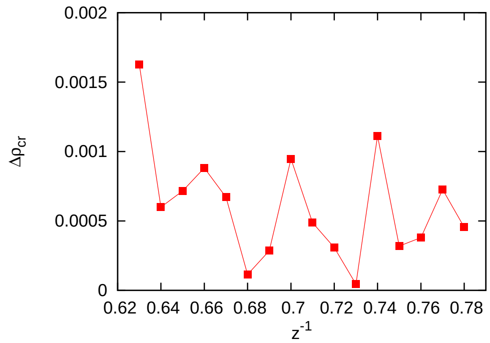

Fig. 5: $\Delta\rho_{\rm cr}$ for z^{-1}.

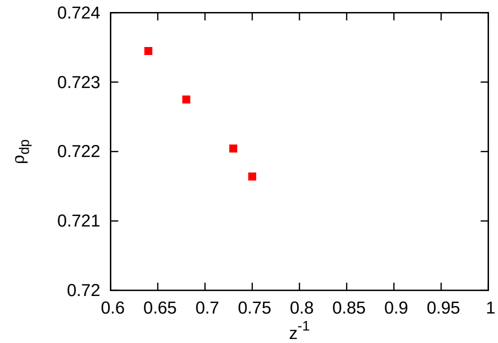

Fig. 6: Dependence of estimated $\rho_{\rm dp}$ for $z^{-1} = 0.64, 0.68, 0.73,$ and 0.75.

and a corresponding dynamical exponent z_*. From numerical experiments, we have $\rho_{\rm dp*} < 0.7217$ and $z_* < 1/0.75$. This result strongly suggests that the freezing transition in our model is not characterized by a combination of exponents of a standard directed percolation, such as the dynamical exponent $z_{\rm dp} \simeq 1/0.63$, unlike in the case of the TBF class [12, 18–20, 22].

Concluding remarks. – The main achievement of this work is the presentation of a direction-free KCM that exhibits a freezing transition on the square lattice. We conjecture by numerical experiments that the singular behaviour at the freezing transition does not belong to the TBF class [12, 18–20, 22]. Lastly, we comment on future studies in the following text.

First, since we have focused on the limiting case $T \to 0$, it is not clear what happens in finite temperature cases. With regard to this problem, we note that the transition point above which frozen particles appear is independent of temperature because it is determined for each initial configuration, while the equilibrium density depends on temperature. Then, if frozen particles are not involved in an equilibrium configuration, the system might not reach the equilibrium configuration and remain trapped in a freezing state. Here, numerical simulations indicate that the fraction of frozen particles changes discontinuously at the transition point and that the fraction above the transition point is always more than 0.5, which is an upper bound of equilibrium densities for any T. Therefore, we conjecture that a freezing transition occurs at the transition point independent of the temperature. This conjecture will be confirmed in a future study.

Second, the characterization of the singular behaviour near the freezing transition in our model remains to be solved. The correct value or more precise estimations for the transition point $\rho_{\rm c}$ and the dynamical exponent z need to be derived theoretically and numerically. In particular, it might be interesting if one explicitly constructs a directed percolation problem related to the behavior near the transition point. Furthermore, the manner of divergence of the relaxation time τ_0 should be clarified. We conjecture that τ_0 in our model exhibits a Vogel-Fulcher type singularity when ρ approaches $\rho_{\rm c}$ from below, in a manner similar to that in the TBF class. Presently, we do not have clear evidence for the conjecture, because $\rho_{\rm c}$ has not been estimated with sufficient accuracy as yet. After obtaining precise estimations for $\rho_{\rm c}$ and z, we will be able to validate our conjecture by numerical experiments.

Third, the theoretical analysis of the model on a Bethe lattice will be performed in order to enhance the understanding of the universality of freezing transitions in KCMs. A concrete question is whether the singular behaviour of the freezing transitions observed here can be characterized by power-law exponents associated with a mode-coupling equation, as discussed in the Fredrickson-Andersen model [15, 23–27]. If the answer is yes, since it is different from the Vogel-Fulcher type singularity, we will clarify the origin of the difference between the behaviours of the model on the Bethe lattice and on the square lattice.

By addressing the points above, we wish to understand how freezing transitions in KCMs are related, or unrelated, to jamming transitions and also wish to establish the universality classes associated with freezing transitions in non-equilibrium phenomena.

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